Hexamethylphosphoramide

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 14.7 °C

Global applicability domain: Inside

Local applicability domain index: 2.83e-01

Confidence level: 3.50e-01

Nearest Neighbors from the Training Set

Image not found
Hexamethylphosphoramide
Measured: 7.20
Predicted: 14.7

Image not found
Boranediamine, 1-fluoro-
N,N,N',N'-tetramethyl-
Measured: -44.3
Predicted: -16.9

Image not found
Tri(aziridin-1-yl)phosphine oxide
Measured: 41.0
Predicted: 44.0

Image not found
Neostigmine methylsulfate
Measured: 143
Predicted: 128

Image not found
Pyridostigmine bromide
Measured: 153
Predicted: 88.2